

Chloroacetic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C8H5Cl3O2/c9-4-8(12)13-5-1-2-6(10)7(11)3-5/h1-3H,4H2
InchiKey: CNALHVZXVPTLGY-UHFFFAOYSA-N
Formula: C8H5Cl3O2
SMILES: O=C(CCl)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 239.48

Physical Properties

Property code	Value	Unit	Source
gf	-160.08	kJ/mol	Joback Method
hf	-286.88	kJ/mol	Joback Method
hfus	25.12	kJ/mol	Joback Method
hvap	59.31	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.138		Crippen Method
mvol	143.980	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
rinpol	1595.00		NIST Webbook
rinpol	1595.00		NIST Webbook
tb	607.66	K	Joback Method
tc	843.00	K	Joback Method
tf	393.30	K	Joback Method
vc	0.546	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.20	J/molxK	607.66	Joback Method
cpg	287.86	J/molxK	646.88	Joback Method
cpg	295.93	J/molxK	686.11	Joback Method
cpg	303.40	J/molxK	725.33	Joback Method
cpg	310.29	J/molxK	764.55	Joback Method
cpg	316.60	J/molxK	803.78	Joback Method
cpg	322.34	J/molxK	843.00	Joback Method
dvisc	0.0012328	Paxs	393.30	Joback Method

dvisc	0.0008286	Paxs	429.03	Joback Method
dvisc	0.0005919	Paxs	464.75	Joback Method
dvisc	0.0004437	Paxs	500.48	Joback Method
dvisc	0.0003456	Paxs	536.21	Joback Method
dvisc	0.0002777	Paxs	571.93	Joback Method
dvisc	0.0002290	Paxs	607.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307716&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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